

Nuclear Octupole Correlations and the Enhancement of Atomic Time-Reversal Violation

J. Engel¹, J.L. Friar², and A.C. Hayes²

¹Department of Physics and Astronomy, CB3255, University of North Carolina,
Chapel Hill, North Carolina 27599

²Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545

February 4, 2008

Abstract

We examine the time-reversal-violating nuclear “Schiff moment” that induces electric dipole moments in atoms. After presenting a self-contained derivation of the form of the Schiff operator, we show that the distribution of Schiff strength, an important ingredient in the ground-state Schiff moment, is very different from the electric-dipole-strength distribution, with the Schiff moment receiving no strength from the giant dipole resonance in the Goldhaber-Teller model. We then present shell-model calculations in light nuclei that confirm the negligible role of the dipole resonance and show the Schiff strength to be strongly correlated with low-lying octupole strength. Next, we turn to heavy nuclei, examining recent arguments for the strong enhancement of Schiff moments in octupole-deformed nuclei over that of ^{199}Hg , for example. We concur that there is a significant enhancement while pointing to effects neglected in previous work (both in the octupole-deformed nuclides and ^{199}Hg) that may reduce it somewhat, and emphasizing the need for microscopic calculations to resolve the issue. Finally, we show that static octupole deformation is not essential for the development of collective Schiff moments; nuclei with strong octupole vibrations have them as well, and some could be exploited by experiment.

1 Introduction

Observation of an atomic electric dipole moment would signal the violation of time-reversal (T) symmetry[1], which kaon decay tells us is present at some level[2]. So far all measurements, whether on elementary particles or atoms and despite rather high sensitivity, have been statistically zero, but experiments continue to improve[3]. The level at which dipole moments are finally seen will help decide among a number of candidates for the fundamental source of T violation.

Several theorists have proposed that the light actinides would be the best elements in which to detect a small dipole moment[4, 5, 6]. Most recently, the authors of refs. [5, 6] have argued that the existence of octupole (pear-shaped) deformation in the nuclei of these atoms enhances the sensitivity of atomic dipole moments to nuclear parity (P) and T violation by factors of 100 to 1000 (typically about 400 in the later reference) over the sensitivity in the atom with the best current experimental limit, ^{199}Hg . This level of enhancement is due in large part to the existence of close-lying parity doublets and favorable atomic structure in the light actinides, but also to fact that it is not the dipole moment of the nucleus that induces a dipole moment in the surrounding electrons, but rather the “Schiff moment”, a quantity that reflects the mean-square radius of the nuclear dipole distribution. Asymmetric nuclei have large intrinsic Schiff moments even though their intrinsic dipole moments are very small, in the same way that a neutral particle can have a finite charge radius.

The arguments of refs. [5, 6] warrant careful investigation. In this paper, we give a pedagogical derivation of the Schiff operator, explore its action on nuclear ground states, and address the role of octupole correlations in generating ground-state Schiff moments. The discussion is organized as follows: section I contains a derivation of the nucleus-electron interaction responsible for atomic-dipole moments and introduces the Schiff operator. The section concludes with an evaluation of the nuclear Schiff moment under the assumption that the dominant source of time-reversal invariance is a nucleon electric dipole moment. Section II reveals important differences between the dipole and Schiff operators, showing that in the Goldhaber-Teller model no Schiff strength is produced by the giant dipole resonance. In section III, we look at Schiff moments in light nuclei, particularly ^{19}F , confirming the near absence of Schiff strength in the giant resonance and pointing out a strong component of strength correlated with low-lying octupole excitations. The first excited state provides the largest contribution to the Schiff moment. Section IV takes up octupole correlations in heavy nuclei, focusing on octupole deformation. We find no flaw in the argument that moments in such nuclei are collective and enhanced, but point to physics that may make the enhancement less dramatic than claimed in refs. [5, 6] (more detailed microscopic calculations of both the octupole-deformed nuclei and those that are currently used in experiments should resolve the uncertainty). In Section V we argue that the collective Schiff moments do not depend on the delicate and sometimes unanswerable question of whether a nucleus is octupole deformed. Low-lying octupole vibrations generate them in the same way as static octupole deformation, increasing the number of atoms in which one can expect large effects. Section VI summarizes our findings.

2 Schiff moments

We begin by deriving the nucleus-electron interaction responsible for generating atomic dipole moments. Though the result is well known[6, 7, 8], a complete derivation has never appeared in one place, and our derivation differs in its details from the others.

In 1939 Feynman[9] developed a quantum theory of molecular forces as part of what is now called the Hellmann-Feynman theorem, or sometimes the parameter theorem. This charming relative of the virial theorem[10] allows insight into how forces in a complex quantum system are balanced against one another, just as they are in a classical system. In a molecule, for example, internal Coulomb forces between electrons and nuclei counter each other so that there is no net force on the molecule (or it would move). In the system we consider here, a neutral atom in a uniform electric field, there is no net charge so there is no net force on the system. To achieve this the electrons rearrange themselves [11] so that there is no net electric field at the nucleus (or it would move).

This shielding effect has dramatic and unfortunate implications for experiments that would probe the atom-nucleus system. Because nuclei are of finite extent, however, the shielding of the electrons varies over the nuclear volume, and this makes probing the nuclear interior possible, as shown originally by Schiff[12]. We present next a variant of Schiff's derivation that uses modern effective-field-theory techniques[13] to produce the simpler approximate result that has been obtained more recently[6, 7, 8].

We assume a neutral (nonrelativistic, for simplicity) atom containing an extremely heavy nucleus with non-vanishing spin sitting in a uniform electric field, \vec{E}_0 . The atom contains Z electrons, each with charge e , while the nuclear charge is Ze_p , where $e_p = -e$ is the proton charge, and in our units the fine-structure constant is given by $\alpha = e_p^2/4\pi$. The nucleus has both an electric monopole distribution and a tiny electric dipole distribution leading to an electric dipole moment $\vec{d} \equiv e_p \vec{d}_0$; other moments can be easily added. In electric-field gauge the atomic-plus-interacting-nucleus Hamiltonian can be written in the form

$$H_{\text{atom}} = \sum_{i=1}^Z \left[K_i + V_i + e\phi(\vec{r}_i) - e\vec{E}_0 \cdot \vec{r}_i \right] - e_p \vec{E}_0 \cdot \vec{d}_0 \quad , \quad (1)$$

where K_i is the kinetic energy of the i^{th} electron ($\vec{p}_i^2/2m_e$ in the nonrelativistic approximation), \vec{r}_i and \vec{p}_i are that electron's coordinate and momentum relative to the nuclear center-of-mass (CM), m_e is the electron mass,

$$V_i = \alpha \sum_{j < i} \frac{1}{|\vec{r}_i - \vec{r}_j|} \quad (2)$$

is the electron-electron Coulomb interaction, and

$$\phi(\vec{r}_i) = \frac{e_p}{4\pi} \int \frac{d^3x \rho(\vec{x})}{|\vec{x} - \vec{r}_i|} \quad (3)$$

is the electrostatic potential due to the complete nuclear charge distribution $\rho(\vec{x})$ (with dimensions ℓ^{-3} , and normalized to Z).

To explore the physics of eq. (1) we employ a trick to remove the last term in that equation. Because $|\vec{d}_0| \equiv d_0$ is tiny even on nuclear scales, it is sufficient to manipulate eq. (1) to first order in that quantity, ignoring all higher-order terms. For example, performing a first-order unitary transformation on H_{atom} produces $\overline{H}_{\text{atom}} \simeq H_{\text{atom}} + i[U, H_{\text{atom}}]$, where $U \sim d_0$ in our case is the Hermitian operator

$$U = \frac{\vec{d}_0}{Z} \cdot \sum_{i=1}^Z \vec{p}_i \quad . \quad (4)$$

Performing the commutator generates two terms, one from the last bracketed term in eq. (1) that cancels the interaction of the nucleus and the external field (U was constructed to do this), and a second that takes its place:

$$\overline{H}_{\text{atom}} = \sum_{i=1}^Z \left(K_i + V_i - e\vec{E}_0 \cdot \vec{r}_i + e\phi(\vec{r}_i) - \frac{e_p}{Z} \vec{d}_0 \cdot \vec{\nabla}_i \phi(\vec{r}_i) \right) \quad . \quad (5)$$

The difference, Δ , between eq. (5) and eq. (1), which cannot lead to an energy shift to first order in d_0 , is given by

$$\Delta = e_p \vec{d}_0 \cdot \left(\vec{E}_0 - \frac{1}{Z} \sum_{i=1}^Z \vec{\nabla}_i \phi(\vec{r}_i) \right) = 0 \quad . \quad (6)$$

This type of relationship, generated by obvious equalities such as $\langle [U, H_{\text{atom}}] \rangle \equiv 0$, is often called a hypervirial theorem[14] and can be derived from the Hellmann-Feynman theorem[9]. If one neglects the finite extent of the nucleus and replaces $\rho(\vec{x})$ by $Z\delta^3(\vec{x})$, eq. (6) can be rearranged into the form

$$\Delta_{\text{point}} = e_p \vec{d}_0 \cdot (\vec{E}_0 + \vec{E}_e) \equiv 0 \quad , \quad (7)$$

where \vec{E}_e is the electric field at the nucleus caused by the electrons. This simple result states that exact screening holds in the point-nucleus approximation, and highlights how a nonzero nuclear volume leads to a small but significant breakdown of screening. Screening is now directly incorporated into $\overline{H}_{\text{atom}}$.

We can now take advantage of the two very different scales — atomic and nuclear — in the Hamiltonian. All of the nuclear physics is contained in $\rho(\vec{x})$ and reflected in $\phi(\vec{r})$; since $(R_N/R_A) \sim (1 \text{ fm}/1 \text{ Å}) \sim 10^{-5}$, only a few moments of $\rho(\vec{x})$ will have practical importance. For this reason we apply a derivative expansion of the type used in effective-field theories[13] to $\rho(\vec{x})$. We assume that the monopole part of $\rho(\vec{x})$ can be expanded in a series of the form: $a\delta^3(\vec{x}) + b\vec{\nabla}^2\delta^3(\vec{x}) + \dots$. An analogous expression holds for the dipole part. For this to make sense the coefficients a, b, \dots together with the derivatives must reflect increasing powers of R_N/R_A . Moreover, we must preserve conventional definitions, such as

$$\int d^3x \rho(\vec{x}) = Z \quad , \quad (8)$$

$$\int d^3x x^2 \rho(\vec{x}) = Z \langle r^2 \rangle_{\text{ch}} \quad , \quad (9)$$

$$\int d^3x \vec{x} \rho(\vec{x}) = \vec{d}_0 \quad , \quad (10)$$

$$\int d^3x \vec{x} x^2 \rho(\vec{x}) = \vec{O}_0 \quad , \quad (11)$$

where the vector quantity \vec{O}_0 [15], which is the second moment of the dipole distribution, bears a similar relationship to \vec{d}_0 as $Z\langle r^2 \rangle_{\text{ch}}$ does to Z . Thus, we posit

$$\begin{aligned} \rho(\vec{x}) &= \left[Z \delta^3(\vec{x}) + Z \frac{\langle r^2 \rangle_{\text{ch}}}{6} \vec{\nabla}^2 \delta^3(\vec{x}) \right] - \left[\vec{d}_0 \cdot \vec{\nabla} \delta^3(\vec{x}) + \frac{\vec{O}_0 \cdot \vec{\nabla}}{10} \vec{\nabla}^2 \delta^3(\vec{x}) \right] + \dots \\ &\equiv \rho_{\text{mon}}(\vec{x}) + \rho_{\text{dip}}(\vec{x}) + \dots \end{aligned} \quad (12)$$

as a sum of monopole and dipole parts. Because derivatives with respect to \vec{x} in ϕ (viz., from ρ) can be transformed into derivatives with respect to \vec{r}_i through integration by parts, this is indeed an expansion in R_N/R_A .

We next separate $\overline{H}_{\text{atom}}$ into a part independent of dipole moments \vec{d}_0 and \vec{O}_0 and another time-reversal- and parity-violating part proportional to these moments:

$$\overline{H}_{\text{atom}} = H_{\text{atom}}^0 + H_{\text{atom}}^{PT} \quad . \quad (13)$$

Expanding $\rho(\vec{x})$ as in eq. (45), we get

$$H_{\text{atom}}^0 = \sum_{i=1}^Z K_i + V_i - e \vec{E}_0 \cdot \vec{r}_i - \frac{Z\alpha}{r_i} + \dots \quad , \quad (14)$$

$$H_{\text{atom}}^{PT} = -\alpha \sum_{i=1}^Z \Delta h(\vec{r}_i) \quad , \quad (15)$$

$$\Delta h(\vec{r}) = \int \frac{d^3x}{|\vec{x} - \vec{r}|} \rho_{\text{dip}}(\vec{x}) + \frac{\vec{d}_0 \cdot \vec{\nabla}}{Z} \int \frac{d^3x}{|\vec{x} - \vec{r}|} \rho_{\text{mon}}(x) \quad . \quad (16)$$

Writing out the explicit expansions for ρ_{mon} and ρ_{dip} leads to the general result for Δh expressed in terms of the Schiff moment[8], \vec{S} :

$$\begin{aligned} \Delta h(\vec{r}) &= 4\pi \vec{S} \cdot \vec{\nabla} \delta^3(\vec{r}) + \dots \\ \vec{S} &= \frac{1}{10} \left[\vec{O}_0 - \frac{5}{3} \vec{d}_0 \langle r^2 \rangle_{\text{ch}} \right] \quad . \end{aligned} \quad (17)$$

Thus, the coupling of the nuclear dipole distribution to the atomic electrons is through the Schiff moment¹. The result (17) depends in leading order on terms of order R_N^3 , because eq. (7) mandates the cancellation of terms of order R_N .

One can make contact with Schiff's paper[12] by defining quantities $\rho_C(x)$ and $\rho_M(x)$ such that $\rho_{\text{mon}}(x)/Z = \rho_C(x)$ and $\rho_{\text{dip}}(\vec{x}) = -\vec{d}_0 \cdot \vec{\nabla} \rho_M(x)$. Equation (10) of ref. [12] then follows from eq. (16) above:

$$\Delta h^{\text{Schiff}}(\vec{r}) = \frac{\vec{d}_0 \cdot \hat{r}}{r^2} \int d^3x (\rho_M(x) - \rho_C(x)) \theta(r - x) \quad . \quad (18)$$

¹The factor of 4π in the first of eqs. 17 is often [3, 7] incorporated in the definition of \vec{S} .

This result is exact but not particularly useful. Expanding ρ_C and ρ_M in the form of eq. (12) leads to the approximate result

$$\Delta h^{\text{Schiff}}(\vec{r}) \simeq \frac{2\pi}{3} \vec{d}_0 \cdot \vec{\nabla} \delta^3(\vec{r}) \left(\langle r^2 \rangle_M - \langle r^2 \rangle_C \right) , \quad (19)$$

from which we deduce the form² of \vec{O}_0 :

$$\vec{O}_0^{\text{Schiff}} = \frac{5}{3} \vec{d}_0 \langle r^2 \rangle_M . \quad (20)$$

Finally, the hypervirial (or Hellmann-Feynman) quantity Δ in eq. (6) can be written using eq. (12) in the form

$$\Delta = e_p \vec{d}_0 \cdot (\vec{E}_0 + \vec{E}_e + \vec{\nabla}^2 \vec{E}_e \frac{\langle r^2 \rangle_{\text{ch}}}{6} + \dots) \equiv 0 , \quad (21)$$

where \vec{E}_e is the electrons' electric field at the nuclear CM, and the last term arises from averaging that electric field over the nuclear volume. Because it is the averaged field that cancels the external field at the nuclear CM, we see explicitly how nuclear finite size affects screening. Moreover, because that last term is equivalent to

$$\frac{2\pi\alpha}{3} \langle r^2 \rangle_{\text{ch}} \sum_{i=1}^Z \vec{d}_0 \cdot \vec{\nabla}_i \delta^3(\vec{r}_i) , \quad (22)$$

we can see that it produces the \vec{d}_0 term in the Schiff moment in eq. (17) (via the second term in eq. (16)). The \vec{O}_0 term in eq. (17) arises from the first term in eq. (16).

Having formulated expressions for nuclear Schiff moments, we want to use them together with assumptions about the dominant source of P and T violation to evaluate Schiff moments in real nuclei. In the rest of this paper we will assume that a P,T-violating component of the nucleon-nucleon interaction causes a Schiff moment in the distribution of protons, but we conclude this section by briefly describing another possibility: that dipole moments of individual nucleons are responsible for the nuclear Schiff moment³.

We introduce proton and neutron (isotopic) projection operators, \hat{p}_i and \hat{n}_i , for the i^{th} nucleon. The dipole moment must point along the spin, $\vec{\sigma}_i$, of the nucleon, leading to the impulse-approximation result[7]

$$\rho_{\text{dip}}(\vec{r}) = \left\langle \sum_{i=1}^A \hat{p}_i d_p \vec{\sigma}_i \cdot \vec{\nabla}_i \rho_{PT}^p(\vec{r}_i - \vec{r}) + \hat{n}_i d_n \vec{\sigma}_i \cdot \vec{\nabla}_i \rho_{PT}^n(\vec{r}_i - \vec{r}) \right\rangle , \quad (23)$$

where ρ_{PT}^p and ρ_{PT}^n are the proton and neutron electric dipole densities (normalized to 1) associated with d_p and d_n . This yields

$$\vec{d}_0 = \left\langle \sum_{i=1}^A (\hat{p}_i d_p + \hat{n}_i d_n) \vec{\sigma}_i \right\rangle \equiv \vec{d}_0^p + \vec{d}_0^n , \quad (24)$$

²This result is a little misleading because it seems to imply that the magnitude of \vec{O}_0 should be d_0 times a typical nuclear size; this need not be the case.

³Meson-exchange currents can also generate P,T-violating nuclear moments directly.

which depends only on the ground-state expectation value of nucleon spin and isospin operators. The Schiff moment can be obtained by evaluating \vec{O}_0 with eq. (23), producing

$$\frac{\vec{O}_0}{10} = \frac{\vec{d}_0^p}{6} \left(\langle r^2 \rangle_{PT}^p + \langle r^2 \rangle_{PT}^Z \right) + \frac{\vec{d}_0^n}{6} \left(\langle r^2 \rangle_{PT}^n + \langle r^2 \rangle_{PT}^N \right) , \quad (25)$$

where $\langle r^2 \rangle_{PT}^p$ and $\langle r^2 \rangle_{PT}^n$ are the mean-square radii of the densities ρ_{PT}^p and ρ_{PT}^n and

$$\left\langle \sum_{i=1}^A \hat{p}_i d_p \vec{\sigma}_i r_i^2 \right\rangle \equiv \vec{d}_0^p \langle r^2 \rangle_{PT}^Z ; \quad \left\langle \sum_{i=1}^A \hat{n}_i d_n \vec{\sigma}_i r_i^2 \right\rangle \equiv \vec{d}_0^n \langle r^2 \rangle_{PT}^N . \quad (26)$$

We expect $\langle r^2 \rangle_{PT}^{Z,N}$ to be comparable to nuclear sizes, and thus much larger than $\langle r^2 \rangle_{PT}^{p,n}$, which should be comparable to nucleon sizes.

3 Distribution of Schiff strength: its significance and the role of the giant dipole resonance

For our considerations, as we have said, the most important mechanism for a nuclear ground-state electric dipole or Schiff moment is the action of a pseudoscalar T-violating nucleon-nucleon potential, \hat{V}_{PT} . This induces a Schiff moment given by second-order perturbation theory:

$$S \equiv \langle S_z \rangle = \sum_{i \neq 0} \frac{\langle \Psi_0 | S_z | \Psi_i \rangle \langle \Psi_i | \hat{V}_{PT} | \Psi_0 \rangle}{E_0 - E_i} + c.c. , \quad (27)$$

where the state $|\Psi_0\rangle$ has $J_z = J \neq 0$ and S_z is the z -component of the Schiff-moment operator \vec{S} . The distribution of Schiff strength to the excited states $|\Psi_i\rangle$ is therefore a crucial ingredient in the ground-state moment. At first sight, one might think that this distribution should resemble that of the electric dipole operator $\vec{r}\tau_z$, but the two are remarkably different. Most of the electric dipole strength is in a broad resonance at 10 to 20 MeV of excitation energy. Almost none of the Schiff strength, however, goes to the states in the giant resonance. In fact, in the simple but venerable Goldhaber-Teller (GT) model, in which the giant dipole resonance corresponds to the $1\hbar\omega$ oscillation of all the protons with respect to all the neutrons, the Schiff strength to the resonance is identically zero.

To see this, we start by assuming[16] rigid distributions for the Z protons and for the N neutrons, which oscillate harmonically about their CM with frequency ω . The separation of the two rigid spherical (for simplicity) distributions is denoted \vec{q} and the distance of the proton CM from the overall CM is $N\vec{q}/A$. The charge distribution is then given by

$$\hat{\rho}_{GT}(\vec{x}) = \rho_0 (|\vec{x} - N\vec{q}/A|) , \quad (28)$$

where ρ_0 is the “bare” nuclear-ground-state charge distribution normalized to Z protons. Expanding this equation, one finds components of $\hat{\rho}_{GT}$ proportional to $|\vec{q}|$, $|\vec{q}|^2$, $|\vec{q}|^3$, \dots ,

or equivalently (because \vec{q} oscillates harmonically), $1\hbar\omega$, 0 and $2\hbar\omega$, 1 and $3\hbar\omega$, etc. In particular one finds that the \vec{q}^2 -term renormalizes the ground-state charge distribution through “vacuum fluctuations” (viz., the *net* $0\hbar\omega$ part, where the nucleus is excited $1\hbar\omega$ and then deexcited by the same amount), a result that we will neglect for the moment since it doesn’t affect the basic physics. Ignoring all but the monopole and dipole parts in eq. (28), we have

$$\hat{\rho}_{\text{GT}} \simeq \rho_0(x) - \frac{N}{A} \vec{q} \cdot \vec{\nabla} \rho_0(x) - \frac{N^3}{10A^3} \vec{q} \cdot \vec{\nabla} \vec{q}^2 \nabla^2 \rho_0(x)|_{3\hbar\omega} + \dots \quad (29)$$

We perform the usual decomposition of \vec{q} in terms of normalized (Cartesian) creation and destruction operators

$$\vec{q} = (\vec{a}^\dagger + \vec{a}) \sqrt{\frac{\hbar}{2\mu\omega}} \quad (30)$$

with

$$[a_i, a_j^\dagger] = \delta_{ij} \quad (31)$$

where $\mu^{-1} = [Zm]^{-1} + [Nm]^{-1}$ is the inverse reduced mass of the (rigid) protons-neutrons system, and m is the nucleon mass.

We discuss the effects of vacuum fluctuations under ref. [17] in the reference list. The only modification they produce is the replacement of ρ_0 in eq. (29) by the complete ground-state charge density of the model, ρ_{ch} . This “renormalization” (removal of the vacuum fluctuations) has for example shifted the $1\hbar\omega$ component of the operator $q^2 \vec{q}$ (the last term in eq. (29)) to the second term of that equation, and only true $3\hbar\omega$ excitations remain from that operator. The modified eq. (29) then expresses the nuclear charge-density operator in terms of the ground-state charge density, the $1\hbar\omega$ transition charge density, the $3\hbar\omega$ (dipole) transition density, etc.

The contribution of the $1\hbar\omega$ excitations to the nuclear moments \vec{d}_0 , and \vec{O}_0 are now easy to obtain. To evaluate the matrix element of the Schiff operator in eq. (27) we need these two moments of the transition charge density, defined by the second term in eq. (29) ($\rho_{\text{dip}}(\vec{x}) = -[N/A] \vec{q} \cdot \vec{\nabla} \rho_{\text{ch}}(x)$ when vacuum fluctuations are included), expressed in terms of \vec{q} , which contains the nuclear raising and lowering operators. One determines the $1\hbar\omega$ components of these moments from eqs. (8-11):

$$\vec{d}_0^{\text{GT}} = \frac{ZN}{A} \vec{q} \quad (32)$$

$$\vec{O}_0^{\text{GT}}(1\hbar\omega) = \frac{5}{3} \vec{d}_0^{\text{GT}} \langle r^2 \rangle_{\text{ch}} \quad (33)$$

The electron-nucleus coupling is defined by $\Delta h(\vec{r})$ in eq. (16). Recalling that ρ_{mon} in that equation is just ρ_{ch} here, and using eq. (32) in ρ_{dip} , we immediately obtain

$$\Delta h_{\text{GT}}(1\hbar\omega) \equiv 0 \quad (34)$$

implying that

$$\vec{S}_{\text{GT}}(1\hbar\omega) \equiv 0 \quad (35)$$

The last conclusion also follows directly from eqs. (33) and (17). Equation (34) is more general than eq. (35), however, because it is true to all orders in R_N/R_A .

Thus, despite the fact that it contains all the dipole strength, the Goldhaber-Teller giant resonance generates no contribution to the Schiff moment and therefore to the atomic dipole moment. In the next section we will see that the same is nearly true in real nuclei.

4 Schiff-strength distributions, octupole correlations, and Schiff moments in light nuclei.

To understand in greater detail the distribution of Schiff strength and the resulting ground-state Schiff moment, we first examine the situation in light nuclei. Although the small radii and charges of light nuclei mean that their Schiff moments will not be large compared to those of heavy nuclei, they have the advantage that their structure can be calculated at a detailed microscopic level.

What kinds of excitations will carry the Schiff strength? We describe elementary excitations in terms of harmonic-oscillator shell-model quanta ($\hbar\omega$); these are not exactly the same as the $\hbar\omega$ of the Goldhaber-Teller model, but the two are related. As shown by Brink[18], the electric dipole operator \vec{d}_0 can excite only those components of the harmonic-oscillator shell-model Hamiltonian (with no residual interactions) corresponding to the giant resonance. That is, the simple $1\hbar\omega$ electric dipole excitations in the harmonic oscillator are exactly the same as in the Goldhaber-Teller model. The operator \vec{O}_0 , on the other hand, can excite other shell-model modes — isoscalar $1\hbar\omega$ and all kinds of $3\hbar\omega$ — that are not a part of the GT model. The GT part of the $1\hbar\omega$ excitations will cancel in \vec{S} as shown above; the isoscalar $1\hbar\omega$ and all $3\hbar\omega$ excitations, by contrast, will contribute to \vec{S} .

Octupole modes are important because the E3 and \vec{O}_0 operators are in some sense the $L = 3$ and $L = 1$ angular-momentum projections of the same operator. The *isoscalar* O_0 and E3 strengths, which contain both $1\hbar\omega$ and $3\hbar\omega$ components, are pulled down into low-lying 1^- and 3^- states (in even-even nuclei) with similar structure. In combination with the suppression of the Schiff strength in the giant-resonance region, this similarity in structure results in most of the available Schiff strength being strongly correlated with octupole excitations. The correlation can be seen in the closed-shell nucleus ^{16}O even without much calculation. The lowest 3^- (6.05 MeV; T=0) state in ^{16}O has an enhanced E3 transition to the ground state, $B(\text{E}3)=13.5\pm0.7$ Weisskopf units (W.u.). The lowest 1^- (7.12 MeV; T=0) state decays to this 3^- state through an enhanced E2 transition, $B(\text{E}2)=21\pm5$ W.u., suggesting that the two states are of similar structure (i.e. that the 1^- state is a quadrupole phonon coupled to the 3^- state). The 1^- state shows an enhanced isospin-forbidden E1 transition to the ground state, $B(\text{E}1)=(3.6\pm0.4)\times10^{-4}$ W.u. Although isospin mixing obviously contributes to the transition, a significant portion of the isospin-forbidden E1 strength appears to come from a large isoscalar matrix element of \vec{O}_0 , a part of the E1 operator that is normally masked[19].

Shell-model calculations reflect the strong correlation between the lowest isoscalar 3^- and 1^- states [20, 21]. Furthermore, the $2p - 2h$ ground-state correlations in such

calculations have a large overlap with the state formed by acting on the closed shell with two successive E3 operators. These higher- $\hbar\omega$ correlations in the ground-state wave function enhance the excitation of octupole-like $3\hbar\omega$ components in the 1^- and 3^- states, leading to larger low-lying isoscalar E3 and \tilde{O}_0 matrix elements.

Let us see how this physics works out in ^{19}F , which has odd A and is therefore able to have a ground-state Schiff moment. The ground state of ^{19}F is the $1/2^+$ head of a $K = 1/2^+(sd)^3$ rotational band, while the first excited state (a $1/2^-$ state at 110 keV) is the basis for a 4p-1h ($p^{-1}(sd)^4$) $K = 1/2^-$ band. SU(3)-basis shell-model calculations[22] for these two bands indicate that the $1/2^-$ band is an octupole excitation of the ground-state band (in fact ^{19}F is considered the closest thing among light nuclei[23] to an octupole-deformed system, though a nonnegligible part of the $1/2^-$ state is an isovector excitation). Though this relation in itself implies large E3 and Schiff matrix elements between these two bands, we have to go beyond these old restricted calculations to get the full picture, for two reasons. First, the just-mentioned octupole ground-state correlations that further enhance the Schiff strength were omitted. Second, we need to ensure realistic behavior for the strength distribution of the P,T-violating NN interaction, which according to eq. (27) is as important as the Schiff-strength distribution in determining the ground-state Schiff moment. Fortunately, its behavior is much simpler. For the sake of pedagogy, we consider in this section a simple but often accurate[24] one-body approximation to \hat{V}_{PT} : $\text{const} \times \vec{\sigma} \cdot \vec{r}$ in both isovector and isoscalar channels (we will use a more sophisticated one-body approximation later). The $1\hbar\omega$ E1 and \hat{V}_{PT} operators then differ only in their effect on spin (they are in the same SU(4) multiplet). The strength from the isovector $\vec{\sigma} \cdot \vec{r}$ is therefore concentrated in an SU(4) analog of the giant dipole resonance, and to first approximation lies at the same energy. The isoscalar strength is also mostly in a resonance at a similar energy, so that low-lying P,T-violating strength is depleted[25]. There will be some strength at low energies where the Schiff strength is concentrated, just as there is some E1 strength, but it will represent the tail of a resonance. This tail was not included in the calculations of ref. [22].

Figures 1-3 display the results of a complete $(0+1)\hbar\omega$ shell-model calculation for ^{19}F , with the center-of-mass motion fully eliminated. In these calculations contributions to the Schiff moment from 2 and $3\hbar\omega$ excitations have been included through the use of an effective charge⁴. Figure 1 shows the isovector O_0 distribution, and above it the isovector S strength. The extent of the cancellation suggested by the Goldhaber-Teller model is remarkable. Also displayed is the isoscalar Schiff strength, which is uncanceled and has a significant low-lying component (again correlated with the E3 distribution). Figure 2 displays the calculated $\vec{\sigma} \cdot \vec{r}$ strength, and the giant resonances (including tails) are evident in both the isovector and isoscalar channels. Finally, in fig. 3 we graph the terms in eq. (27) as a function of excitation energy, assuming that the isoscalar and isovector potentials have equal strength; from this it is clear that the lowest $1/2^-$ state almost

⁴It is difficult to treat the important $2\hbar\omega$ and $3\hbar\omega$ excitations consistently in the low-lying states. However, the concept of an effective charge for E3 transitions works well throughout this mass region. The results of very truncated $(0+1+2+3)\hbar\omega$ calculations suggest a similar prescription for the \tilde{O}_0 operator, and in our $1\hbar\omega$ calculations we applied octupole effective charges to \tilde{O}_0 . Reference [19] makes a case for this same kind of renormalization.

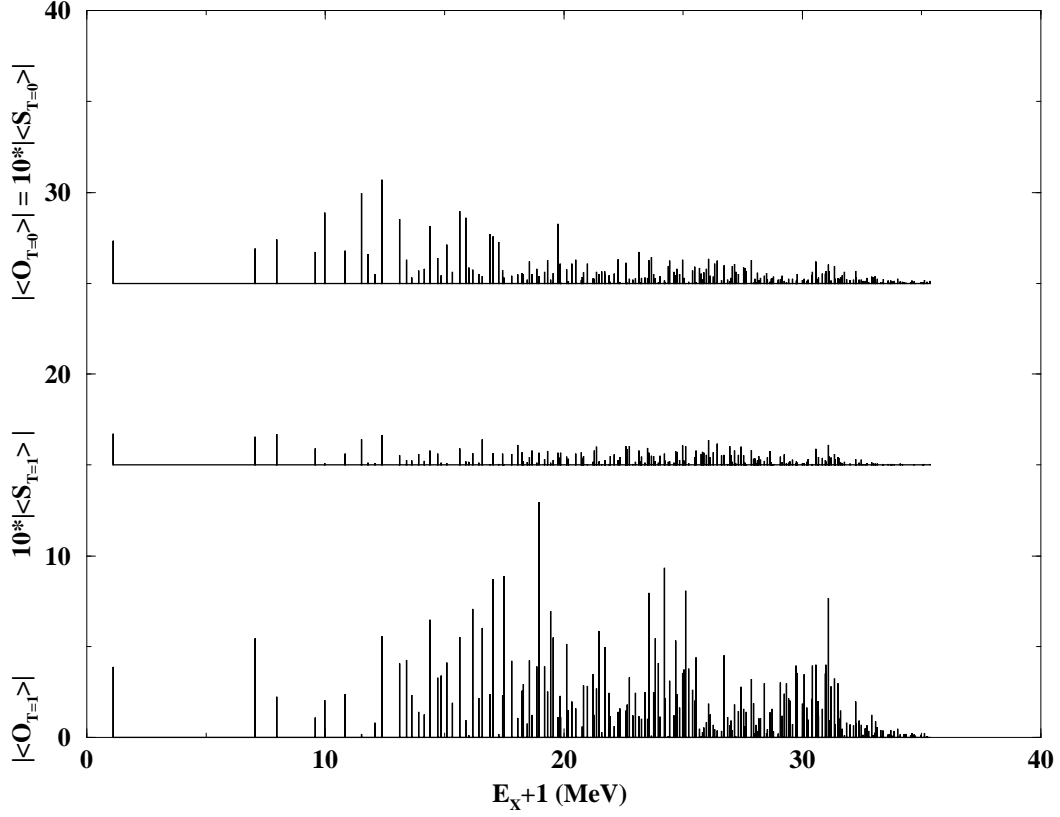


Figure 1: The distribution of isovector O_0 strength (bottom), isovector Schiff strength (middle) and isoscalar Schiff ($\propto O_0$) strength (top) in a shell-model calculation of ^{19}F . See text for discussion.

completely determines the Schiff moment, which is given by the sum of all the lines in the plot.

We expect the gross features of the Schiff and V_{PT} distributions to be general. The Schiff strength will be correlated with the E3 strength and lie low in energy. Nuclei with octupole deformation, where the E3 strength lies as low as ~ 50 keV and is particularly concentrated, will show the most-enhanced Schiff moments. Nuclei with strong low-lying octupole vibrations should also show enhancement. As the E3 strength moves up in energy (and/or the octupole collectivity is diluted), so should the dominant contribution to the Schiff strength, and the Schiff moments will become smaller. In the remainder of this paper we examine the extent to which these statements are true in heavy nuclei, where shell-model calculations are not possible.

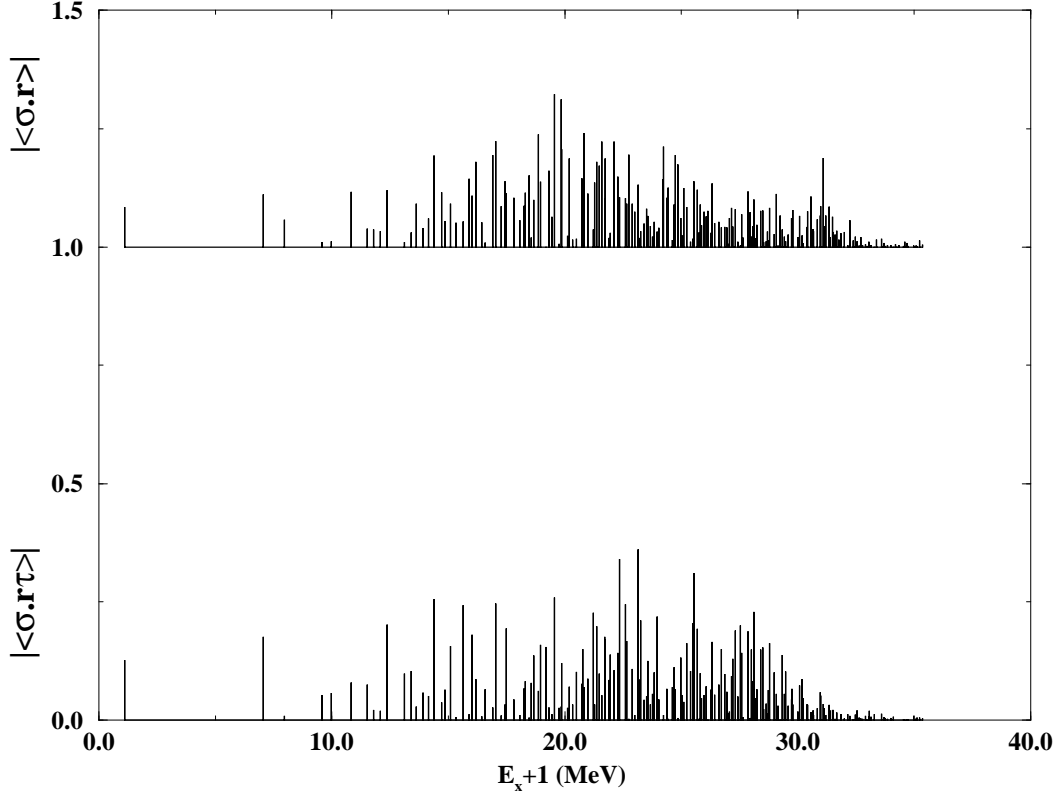


Figure 2: Distributions of the isovector (bottom) and isoscalar (top) $\vec{\sigma} \cdot \vec{r}$ strengths in ^{19}F . The corresponding operators are approximations to the P,T-violating nuclear potential.

5 Collective Schiff moments in heavy octupole-deformed nuclei.

We begin our discussion with a short review of the arguments of ref. [6], the crux of which is related to what we have already discussed: the ground-state Schiff moment need not be directly related to the dipole moment, and in the case of octupole-deformed nuclei is considerably more enhanced. The authors adopted the particle-rotor model, which is not fully microscopic and omits a certain amount of valence-space physics. The arguments are based on collective octupole correlations, however, and this model represents them clearly and efficiently.

In the particle-rotor model the nucleus is described as a single particle coupled to a collective core, the shape of which can be specified through a function that describes the dependence of its radius on angle:

$$R(\theta, \phi) = R_0 \left(1 + \sum_{l,m} (-1)^m \alpha_{l,m} Y_{l,-m} \right) , \quad (36)$$

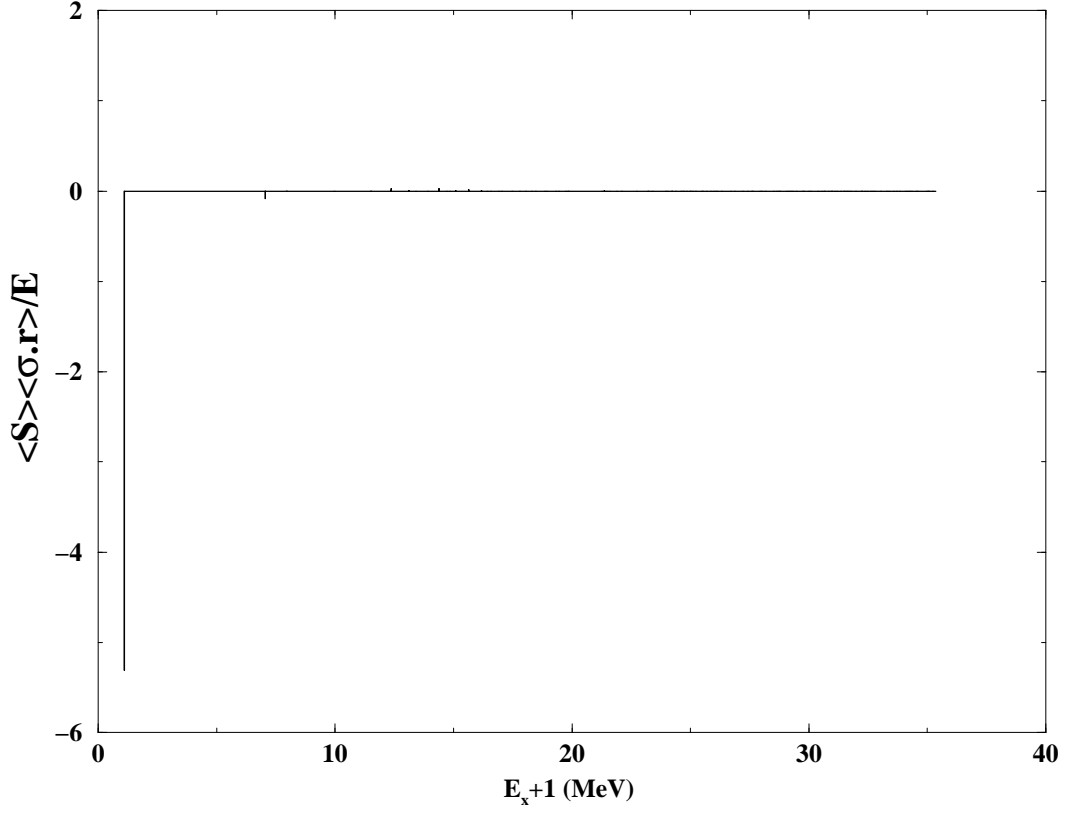


Figure 3: The contributions of individual states in ^{19}F to the ground-state Schiff moment through eq. (27). The first excited state is dominant.

where $R_0 = 1.2A^{1/3}$. In the intrinsic frame of a deformed nucleus three of the α variables are no longer independent; they are replaced by three Euler angles θ_i ($i = 1, 2, 3$) that specify the orientation with respect to the laboratory. We will assume axial symmetry so that all intrinsic α 's vanish except for the $\alpha_{l,0}$'s, which we denote by β_l . The valence particle, in the “strong-coupling” version of the model, moves in a potential that is deformed to match the shape of the core. The full nuclear wave function (for a state with angular momentum quantum numbers J and M , intrinsic magnetic quantum number K , and parity p) thus depends on the Euler angles, the intrinsic deformation parameters β_l , and the intrinsic space (\vec{r}) and spin (s) coordinates of the odd particle:

$$\langle \theta_i, \beta_l, \vec{r}, s | \Psi_{JMK,p} \rangle = \mathcal{N} \left[1 + \hat{R}_2 \right] D_{MK}^{J*}(\theta_i) \left[1 + p\hat{P} \right] \langle \beta_l, \vec{r}, s | \Psi_{\text{int}} \rangle, \quad (37)$$

where the intrinsic particle-core state factorizes as⁵

$$\langle \beta_l, \vec{r}, s | \Psi_{\text{int}} \rangle = \Phi(\beta_l) \psi_K(\vec{r}, s). \quad (38)$$

⁵In axially symmetric nuclei, the component K of total angular momentum along the symmetry axis is equal to that of the particle's angular momentum (sometimes denoted Ω).

Here \mathcal{N} is a normalization constant, \hat{R}_2 rotates the D -functions and the intrinsic wave function by 180 degrees around the y -axis, and \hat{P} changes the sign of \vec{r} and of the odd-multipole β_l 's in the intrinsic wave function. As long as we do not allow nonaxial core vibrations to be excited, we can, for the purposes of this paper, write the Schiff operator S_z as

$$S_z = D_{00}^{1*}(\theta_i) \hat{S}_{\text{int}}(\hat{\beta}_l, \vec{r}, \vec{\sigma}) , \quad (39)$$

where \hat{S}_{int} is the intrinsic-frame operator, with only the $K = 0$ component relevant because others do not generate collective excitations in the absence of nonaxial deformation or vibration. [For \hat{V}_{PT} , the transformation to the intrinsic frame is trivial because that operator is invariant under rotation.] We have placed hats on the β 's and (on S_{int}) because at the quantum level they are operators that act on the wave functions $\Phi(\beta_l)$ in eq. (38). All of this formalism can be justified at least in part through projected mean-field calculations, in which the state is a function of all A nucleon coordinates; we will argue shortly that such calculations are necessary to answer questions that arise in the simpler description.

In the simple particle-rotor model, matrix elements of one-body operators like S_z are straightforward to calculate. The coordinates of the individual nucleons in the core are integrated over in the intrinsic frame to give an operator that is a function of the collective coordinates and those of the odd particle, and can be applied to wave functions of these same coordinates. When one does the integration for the Schiff operator, assuming a nuclear charge density proportional to the mass density (so that the intrinsic dipole moment is zero⁶), the result is

$$\hat{S}_{\text{int}} = ZeR_0^3 \frac{3}{20\pi} \sum_{l=2} \frac{(l+1)\hat{\beta}_l\hat{\beta}_{l+1}}{\sqrt{(2l+1)(2l+3)}} + S_{\text{int}}(\text{s.p.}) , \quad (40)$$

where the last term is the contribution of the valence particle, which in this case can be neglected compared to the collective piece. Without the hats, the first term in eq. (40) is just the classical Schiff moment of a deformed drop.

Interesting things happen when a core is both quadrupole and octupole deformed (i.e. when $\Phi(\beta_l)$ is peaked around nonzero values of β_2 and β_3). [For a comprehensive review of the subject, see ref. [23].] The reflection asymmetry implies a double-well potential in the coordinate β_3 , which in turn means that the wave functions with good parity will be linear combinations of functions peaked around some β_3 and its negative. If the barrier between the two wells is high enough, the result will be parity-doubling; low-lying states will have partners nearby with the same angular momentum but opposite parity. This means, for one thing, that there will be an intermediate state in (27) that enters with a small energy denominator and therefore a large amplitude. In fact, it is often reasonable to ignore all other states in the sum (see the shell-model result for ^{19}F in fig. 3), mainly because of the energy denominator, but also because if the deformation is strong enough the matrix element of the Schiff operator to that state is likely to be large. The reason

⁶The collective contribution to the dipole moment is obviously hard to calculate precisely if in this approximation it is identically zero.

for that is that the doublets can be viewed as the projection onto positive and negative parity of the same reflection-asymmetric intrinsic state $|\Psi_{\text{int}}\rangle$.

The existence of more than one state with the same intrinsic structure is exactly the same phenomenon as the rotational bands associated with ordinary reflection-symmetric deformation. The matrix element of an operator between the two states of the same doublet is proportional to the diagonal intrinsic-state matrix element of the intrinsic operator, just as it is for states within a rotational band. For the operator \hat{S}_{int} , this diagonal matrix element is large; it is given roughly by the expression in eq. (40) with the operators $\hat{\beta}_l$ replaced by the values around which the wave function $\Phi(\beta_l)$ is peaked (i.e. by the classical Schiff moment of the deformed asymmetric core), with coherent contributions from all the nucleons in it⁷. Thus, from eq. (27), the physical ground-state Schiff moment S that determines the atomic electric dipole moment should be approximately

$$S \approx -2 \frac{J}{J+1} S_{\text{int}} \frac{\langle \tilde{\Psi}_0 | \hat{V}_{PT} | \Psi_0 \rangle}{\Delta E}, \quad (41)$$

where $|\tilde{\Psi}_0\rangle$ is the opposite-parity partner of the ground state $|\Psi_0\rangle$, ΔE is the energy difference between the two states, and S_{int} is the intrinsic Schiff moment (the J -dependent factor is from the Euler-angle integration). The conclusion from all this is that large intrinsic Schiff moments and small energy denominators should make atoms with octupole-deformed nuclei especially sensitive tests of P,T-violation in the nucleon-nucleon interaction.

Just how sensitive the tests will be depends on the matrix element of the interaction \hat{V}_{PT} , to which we now turn. We will supply more detail in addressing this subject because the treatment of ref. [6] is incomplete and not entirely accurate. We assume that the pion is responsible for transmitting most of the T-violating force from one nucleon to another [24]. The nucleon-nucleon interaction produced by one-pion exchange then has the general form[4, 26]

$$\begin{aligned} \hat{V}_{PT}(12) &= \left\{ \begin{aligned} &(\vec{\sigma}_1 - \vec{\sigma}_2) \cdot (\vec{r}_1 - \vec{r}_2) [C_0 \vec{\tau}_1 \cdot \vec{\tau}_2 + C_1(\tau_{1z} + \tau_{2z}) + C_2(3\tau_{1z}\tau_{2z} - \vec{\tau}_1 \cdot \vec{\tau}_2)] \\ &+ C_1(\vec{\sigma}_1 + \vec{\sigma}_2) \cdot (\vec{r}_1 - \vec{r}_2)(\tau_{1z} - \tau_{2z}) \end{aligned} \right\} \\ &\times \frac{\exp(-m_\pi |\vec{r}_1 - \vec{r}_2|)}{m_\pi |\vec{r}_1 - \vec{r}_2|^2} \left[1 + \frac{1}{m_\pi |\vec{r}_1 - \vec{r}_2|} \right], \end{aligned} \quad (42)$$

where the C_i 's label isoscalar, isovector, and isotensor contributions. As long as we excite no particles out of the core, P,T-violating interactions between these particles sum to zero (see ref. [6] for discussion), and we need worry only about the interactions between the valence particle and those in the core. In what follows, we take the total mass density to be proportional to the charge density, and in fact *from now on use the symbol ρ to represent the mass density*. This assumption means that the terms with different isospin structure in eq. (42) enter in similar ways. Taking the range of the pion to be very short (a decent approximation[25]), summing eq. (42) over the particles in the core, and assuming

⁷As pointed out in refs. [5] and [6], the collective enhancement of the dipole moment is much smaller (zero in fact if the charge distribution is proportional to the mass distribution) because the dipole moment is measured from the center of mass.

the neutron and proton densities to be equal gives the effective nucleon-core interaction

$$\hat{U}_{PT} = \eta \frac{G}{2m\sqrt{2}} \vec{\sigma} \cdot \vec{\nabla} \hat{\rho} , \quad (43)$$

where (again) $\hat{\rho}$ is the core mass-density operator, G is the Fermi constant, and m is the nucleon mass (these factors are inserted to follow convention). The dimensionless parameter η then depends on the coupling strengths C_i of the two-body interactions and the isospin of the nucleus. Despite its slight dependence on nuclear structure, this parameter is often taken as a “heuristic” fundamental quantity. The one-body approximation given by eq. (43) is slightly different from the simpler and more phenomenological one we used in our discussion of light nuclei.

The form of eq. (43) makes the Schiff moment unpleasantly sensitive to the distribution of spin near the nuclear surface, where $\vec{\nabla} \rho$ is largest. The results of ref. [6] sometimes differ by factors of several from those of ref. [5], primarily because of differences in the valence single-particle wave function, which carries all the nuclear spin \vec{s} in the particle-rotor model. Only a significantly more sophisticated calculation (which we advocate) will reduce this uncertainty. We therefore do not present our own complete “particle-rotor-model-with-octupole-deformation” calculations in this section, but instead use that model in its simplest form, together with qualitative arguments, to identify a few systematic effects overlooked in the existing calculations. Our estimate of the size of these effects is obviously uncertain, but indicates what can be expected in more sophisticated calculations. The new physics always tends to lessen the enhancement.

To see the what was neglected in refs. [5, 6] we follow ref. [27] and expand the density in the deformation parameters:

$$\begin{aligned} \rho(\vec{r}) &\approx \rho_0(r - R(\theta, \phi) + R_0) \\ &\approx \rho_0(r) - R_0 \rho'_0(r) \sum_l \beta_l Y_{l,0} + 1/2 R_0^2 \rho''_0(r) (\sum_l \beta_l Y_{l,0})^2 + \dots , \end{aligned} \quad (44)$$

where now $\rho_0(r)$ is the bare (spherical) ground-state mass density of the core, a constant up to radius R_0 in the simplest version of the liquid-drop picture. The operator $\vec{\sigma} \cdot \vec{\nabla} \hat{\rho}$ in \hat{U}_{PT} therefore depends on the $\hat{\beta}$ ’s, and, contrary to the statements in ref. [6], cannot be broken up into pseudoscalar pieces that act separately on the core and particle. In fact, from eq. (44) we have

$$\begin{aligned} \vec{\sigma} \cdot \vec{\nabla} \hat{\rho} &= \vec{\sigma} \cdot \vec{\nabla} \rho_0 \\ &+ R_0 \sum_l \hat{\beta}_l \left[\sqrt{\frac{l+1}{2l+1}} \left(\frac{d}{dr} - \frac{l}{r} \right) \rho'_0[Y_{l+1}\sigma]_0^l - \sqrt{\frac{l}{2l+1}} \left(\frac{d}{dr} + \frac{l+1}{r} \right) \rho'_0[Y_{l-1}\sigma]_0^l \right] \\ &- 1/2 R_0^2 \sum_{l,l',L} \hat{\beta}_l \hat{\beta}_{l'} \sqrt{\frac{(2l+1)(2l'+1)}{4\pi(2L+1)^2}} \langle l0, l'0 | L0 \rangle \\ &\times \left[\sqrt{L+1} \left(\frac{d}{dr} - \frac{L}{r} \right) \rho''_0[Y_{L+1}\sigma]_0^L - \sqrt{L} \left(\frac{d}{dr} + \frac{L+1}{r} \right) \rho''_0[Y_{L-1}\sigma]_0^L \right] , \end{aligned} \quad (45)$$

where the small square brackets indicate angular-momentum coupling. Reference [6] considers only the first term in this expression, which changes the parity of the single particle and leaves the core alone. The terms with odd powers of $\hat{\beta}_3$ can do the opposite, however.

Including these other terms is important because in the strong-coupling limit of the particle-rotor model they tend to cancel the first term. The reason is hinted at in ref. [6], where it is argued that Schiff moments between close-lying states are suppressed when deformation is rigid and symmetric. Following ref. [8], the authors note that to the extent that the density is proportional to the strong one-body potential \hat{U}_{strong} felt by the odd particle and that the spin-orbit force is negligible, matrix elements of $\vec{\sigma} \cdot \vec{\nabla} \hat{\rho}$ between two states should be proportional to the energy difference between those states, and therefore very small for close-lying doublets. The reason is that under these circumstances

$$\vec{\sigma} \cdot \vec{\nabla} \hat{\rho} \propto \vec{\sigma} \cdot \vec{\nabla} \hat{U}_{\text{strong}} = i[\vec{\sigma} \cdot \vec{p}, \hat{U}_{\text{strong}}] = i[\vec{\sigma} \cdot \vec{p}, \hat{H}(\text{s.p.})] , \quad (46)$$

so that for two opposite-parity states labeled a and b with the same core structure,

$$\langle \Psi_{JMK,p}^a | \hat{U}_{PT} | \Psi_{JMK,-p}^b \rangle \propto \langle \psi_{a,K} | \vec{\sigma} \cdot \vec{\nabla} \rho | \psi_{b,K} \rangle \propto \epsilon_a - \epsilon_b , \quad (47)$$

where the ϵ 's are single-particle energies. The authors then argue that complications associated with asymmetric deformation eliminate this effect, but in the strong-coupling limit the situation is even worse because now the two states $|\Psi_{JMK,p}^a\rangle$ and $|\Psi_{JMK,-p}^b\rangle$ have the same intrinsic structure. As mentioned above, the matrix element of any operator between two such states is proportional in the strong-coupling limit to the intrinsic-state expectation value of the operator. In nuclei with strong octupole deformation, we therefore have

$$\langle \Psi_0 | \hat{V}_{PT} | \tilde{\Psi}_0 \rangle \longrightarrow \langle \Psi_{\text{int}} | \hat{U}_{PT} | \Psi_{\text{int}} \rangle = \eta \frac{G}{2m\sqrt{2}} \langle \psi_K | \vec{\sigma} \cdot \vec{\nabla} \rho | \psi_K \rangle , \quad (48)$$

which, according to the argument above, should vanish. The estimates of refs. [5, 6] apparently neglect the terms in ρ containing the β 's that make the shapes of the density distribution and the potential similar, and so do not take this effect into account.

Of course the spin-orbit force is not negligible and the intrinsic density is not exactly proportional to the mean field, so the cancellation will not be complete. To get a handle on how much the terms containing the β 's affect the matrix element of \hat{U}_{PT} , we consider the ratio of the matrix element in eq. (48) with the terms included to that without them (the latter being a simplified version of the quantity calculated in refs. [5, 6]) for a large number of single-particle orbits. We use a deformed harmonic oscillator as a potential,

$$V(\vec{r}) = -m\omega r^2 \sum_l \beta_l Y_{l,0} , \quad (49)$$

with deformations β_2 , β_3 , and β_4 equal to those from Table I of ref. [6] (we ignore higher multipoles and neglect pairing). We take the density to be constant inside the liquid drop and zero outside, a distribution that has the same angular shape as the potential, but a significantly different radial dependence. Figure 4 shows the absolute value of the ratio of $\langle \psi_K | \vec{\sigma} \cdot \vec{\nabla} \hat{\rho} | \psi_K \rangle$ to the same matrix element without the β -dependent terms, for all $K = 1/2$ and $K = 3/2$ single-particle levels in ^{225}Ra below $8 \hbar\omega$ of single-particle

energy. The new terms generally have the opposite sign from that of the β -independent term, and the sum is usually less than the first term by itself. The average cancellation is less for $j = 1/2$ states than for states with larger spin. Whether the decrease will be stronger or weaker in realistic calculations is an open question. In self-consistent mean-field calculations, though, there is obviously a correlation between the density and the spin-independent part of the field, and we could well see a significant effect⁸.

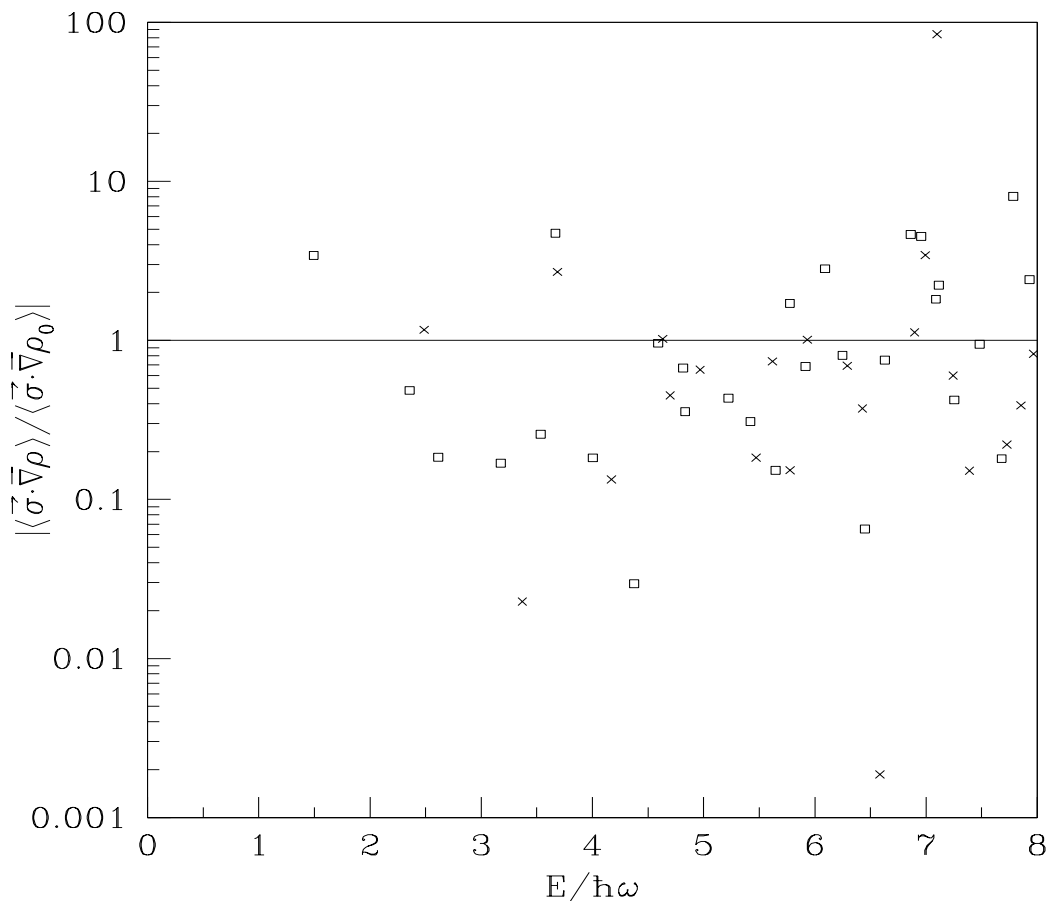


Figure 4: The ratio $|\vec{\sigma} \cdot \vec{\nabla} \rho|$ to $|\vec{\sigma} \cdot \vec{\nabla} \rho_0|$ (see text) for all $K = 1/2$ (boxes) and $3/2$ (crosses) states in a deformed asymmetric potential for ^{225}Ra . The ratio is usually less than one.

Other physics neglected in the earlier work will also have an effect. The first term in eq. (45) ($\vec{\sigma} \cdot \vec{\nabla} \rho_0 = (1/r) \rho'_0 \vec{\sigma} \cdot \vec{r}$) is the spin-flip analog of the electric dipole operator (with a difference only in radial form and isospin). We refer to fig. 2, where the strength of the related operator $\vec{\sigma} \cdot \vec{r}$ in the isovector and isoscalar channels is plotted for ^{19}F . As noted in section III, the strength is clearly concentrated in resonances at about the same energy as

⁸We should add that the decoupling of the particle and core[33], taken into account neither here nor in ref. [6], could act like the spin-orbit interaction to mitigate the suppression.

the giant dipole resonance. A simple argument[28] with a schematic residual interaction in RPA shows that the existence of the giant dipole resonance of the core suppresses E1 transitions between low-lying single-particle states by a factor of 3 or 4 that depends only on the energy of the resonance and the energy at which strength would be centered if there were no resonance. The low-lying transitions induced by $\vec{\sigma} \cdot \vec{\nabla} \rho_0$ should be suppressed by roughly the same amount because the operator $\vec{\sigma} \cdot \vec{r}$ is so much like \vec{r} (again, see fig. 2). In many-body perturbation theory, this effect can be understood as core polarization: the residual strong interaction can create a collective 0^- p-h pair, at the same time changing the parity of the valence particle. The contribution to the Schiff moment coming from the annihilation of the pair by \hat{U}_{PT} nearly cancels the contribution coming from the direct action of \hat{U}_{PT} on the valence particle itself. In any event, the resonances were completely neglected in refs.[5, 6], and the single-particle matrix elements in those papers should therefore probably be three or four times smaller.

The very large Schiff moments may be saved, however, by the *combination* of the two new effects, even though each reduces Schiff moments when added to the calculations of refs. [5, 6] in isolation. The spin-flip giant resonance should not affect those parts of \hat{U}_{PT} that contain β_3 and operators like $[Y_2\sigma]_0^3$ that do not change the parity of the valence particle. The suppression by the residual interaction of one part of the Schiff moment by a factor of three without any effect on another part may upset any balance between the two at the mean-field level produced by the similarity between the density and the potential. We will need accurate microscopic calculations to test the existence of both effects and the extent to which they offset one another.

Such calculations are within the range of today's mean-field technology, and in even-even nuclei they have already been carried out[29, 30], confirming the large intrinsic Schiff moments in the radium isotopes[31]. In self-consistent (e.g. Skyrme-HFB) calculations the effects of the residual interaction on the ground state are minimized. Therefore, not only is the relationship between the mean field and the density likely to be most accurate in this case, but it is also least likely to be vitiated by corrections to the single-particle picture. In odd nuclei, the first-order core polarization, which has to be treated as a correction to particle-rotor/Nilsson models, is built into the mean-field; 1-particle-1-hole excitations of the core do not mix with the ground state. This fact, together with a realistic two-body interaction that contains all multipole-multipole terms, has implications for corrections to low-lying transitions from resonances, as well as for the density. The incorporation of core polarization means that the interplay between collective excitations and low-lying states is already apparent at the mean-field level, or in other words that the usual first-order particle-phonon mixing that reduces low-lying single-particle transitions need not be treated by other means (e.g. the RPA). We should therefore be able at the mean-field level to go a long way towards quantifying the influence of shape and resonances on Schiff moments in octupole-deformed nuclei.

6 Collective Schiff moments from octupole vibrations

The question of whether the light actinides are octupole deformed has a long history. In

fact the question is not entirely physical — it's really about the economy of one collective-model basis versus another — and it should not matter so much whether the low-lying states in a nucleus are best described as the rotation of an octupole-deformed shape or as a strong low-lying octupole vibration around a rotating quadrupole shape. Collective Schiff moments arise in either scheme. This fact should not be surprising in light of our calculations in ^{19}F . To see how it falls out of the collective picture, we assume that the nuclear core has no equilibrium octupole deformation (i.e. $\langle\beta_3\rangle = 0$) and write the operator $\hat{\beta}_3$ in terms of creation and annihilation operators:

$$\hat{\beta}_3 \propto b^\dagger + b, \quad (50)$$

where b^\dagger creates an octupole phonon with (intrinsic) magnetic quantum number $K = 0$. It is then clear from eq. (40) that the Schiff operator acting on a quadrupole-deformed state with no octupole phonons will create an excited state with one phonon. The terms in \hat{U}_{PT} (see eq. (45)) that are proportional to $\hat{\beta}_3$ can then destroy the phonon, reconnecting the one-phonon state to the ground state and generating a collective Schiff moment through eq. (27).

To see how big such a moment would be we need to know the matrix element of $\hat{\beta}_3$ between states with zero and one phonons. As can be seen from eq. (50), this quantity is just the zero-point root-mean-square deformation, $(\sqrt{\langle\hat{\beta}_3^2\rangle})$, which we will call $\bar{\beta}_3$. [In other words, $\bar{\beta}_3$ measures the spread in β_3 of the intrinsic core wave function $\Phi(\beta_l)$.] This quantity can be estimated from the collective (vibrational) B(E3) transition in an even-even neighbor. Using eq. (44) to lowest order in $\bar{\beta}_3$ one finds[32]

$$B(E3)_{0^+ \rightarrow 3^-} = (3/4\pi)^2 (ZeR_0^3)^2 \bar{\beta}_3^2. \quad (51)$$

The important point is that if a collective vibration is soft the r.m.s. deformation $\bar{\beta}_3$ can be as large as the value around which the wave-function is peaked in octupole-deformed nuclei, and the intrinsic Schiff moment can therefore be just as large as well. In the laboratory (physical) Schiff moment, there is an additional factor of $\bar{\beta}_3$ coming from the annihilation of the phonon by \hat{U}_{PT} , so that naively we expect the moment to depend on the deformation parameters in the combination $\beta_2 \bar{\beta}_3^2$, where an unbarred β is the value around which the deformed wave function is peaked. The relevant quantity for octupole-deformed nuclei is $\beta_2 \beta_3^2$ (see ref. [6] for a discussion of why), so that if the r.m.s. octupole deformation $\bar{\beta}_3$ in a vibrational nucleus is comparable to the static value β_3 of the deformation in an octupole-deformed nucleus, any differences in Schiff moments come from the energy denominator, single-particle structure, or other core excitations, not from the difference between deformation and vibration. We will refine this statement shortly.

First, however, we note that the terms in \hat{U}_{PT} that don't contain $\hat{\beta}_3$ are usually even more important than those just discussed, even though they don't alter the number of phonons, because the zero- and one-phonon states mix through the residual strong particle-core interaction. The approximate form of this coupling can be derived in many ways; one is to examine the change in energy under a small deformation of the core. Not surprisingly, for an oscillator single-particle potential this leads to the same interaction that appears in

the octupole-deformed potential of the strong-coupling scheme (see eq. (49):

$$\hat{V}_{\text{coupl}} = -m\omega^2 \hat{\beta}_3 r^2 Y_{3,0} , \quad (52)$$

where ω is the oscillator energy of the (symmetric) potential, $\hat{\beta}_3$ acts on the core, and $r^2 Y_{3,0}$ acts on the particle. Denoting a state with n phonons and a particle in orbit $\psi_{a,K}^p$ by $|n, \psi_{a,K}^p\rangle$, we have for the matrix element of the interaction \hat{V}_{coupl} between excited states with one phonon and the unperturbed ground state (assuming just for illustration that the ground state has positive parity):

$$\langle 1, \psi_{b,K}^- | \hat{V}_{\text{coupl}} | 0, \psi_{a,K}^+ \rangle = -m\omega^2 \bar{\beta}_3 \langle \psi_{b,K}^- | r^2 Y_{3,0} | \psi_{a,K}^+ \rangle . \quad (53)$$

With a value for $\bar{\beta}_3$ from an appropriate $B(E3)$, we can use the “intermediate”-coupling scheme of ref. [33] to diagonalize $\hat{H} \equiv \hat{H}(\text{s.p.}) + \hat{H}(\text{phonon}) + \hat{V}_{\text{coupl}}$ separately in positive- and negative-parity bases ($\hat{H}(\text{phonon})$ just contains the diagonal vibrational energies of the zero- and one-phonon states), so that the ground state has the form

$$|\Psi_0\rangle = \sum_i A_i |0, \psi_{i,K}^+\rangle + \sum_j B_j |1, \psi_{j,K}^-\rangle , \quad (54)$$

and the excited states of opposite parity have the form

$$|\Psi_l\rangle = \sum_i C_{l,i} |1, \psi_{i,K}^+\rangle + \sum_j D_{l,j} |0, \psi_{j,K}^-\rangle , \quad (55)$$

where the $\psi_{i,K}^+$ and $\psi_{j,K}^-$ label single-particle states around the Fermi surface, and we are still ignoring nonaxial vibrations. The terms in \hat{U}_{PT} that are independent of $\hat{\beta}_3$ connect the first terms in eq. (54) to the second in eq. (55) and vice versa. The Schiff operator affects the core, connecting the first term in eq. (54) to the first in eq. (55), and the second to the second, effectively replacing $\hat{\beta}_3$ in eq. (40) by $\bar{\beta}_3$. In this way the spherical $\hat{\beta}_3$ -independent part of \hat{U}_{PT} (the only part considered in refs. [5, 6]) can also generate a collective Schiff moment.

It is possible to use the intermediate-coupling scheme even as the phonon energy goes to zero and octupole deformation sets in. In that case, because the single-particle Hamiltonians in the two schemes are the same, energies and matrix elements should not depend strongly on which scheme is used⁹. One implication (which is a stronger version of a remark made above) is that if the dynamic $\bar{\beta}_3$ associated with the vibration is comparable to the static β_3 in an octupole-deformed nucleus, and if the energy of the octupole phonon is small compared to typical single-particle splittings or nonaxial core-excitation energies, the *only* major difference between Schiff moments in the two cases is the energy denominator in eq. (27). To see this, one can imagine treating the phonon as a “decoupling” perturbation (along with the Coriolis interaction) in the strong-coupling scheme, as is done in ref. [33]. Although the diagonal matrix elements of the perturbation cause energy

⁹They will not be identical because in the intermediate-coupling scheme some of the states are particles and some holes, and single-particle excitation energies are measured with respect to the Fermi surface[33].

shifts, wave functions are only affected by the off-diagonal matrix elements with bands built on higher single-particle states or other kinds of vibrations. Thus wave functions, transition amplitudes, etc., will not undergo large changes until the energy of the phonon approaches those of other excitations. For the intermediate-coupling scheme, this means that the matrix elements of S and \hat{V}_{PT} connecting ground states to low-energy octupole phonons should not undergo radical change once the phonon is low enough in energy, and that nothing special will happen in the limit that the phonons have zero energy and the core develops static deformation. Of course if the phonon lies high in the spectrum, the matrix elements can be very different from the static limit, and one must carry out the intermediate-coupling calculation to get a handle on the size of the Schiff moment induced by vibrations.

We have done just that in several quadrupole-deformed nuclei, taking vibrational $\bar{\beta}_3$'s and phonon energies from tabulations of nearby even-even nuclei[32], and again neglecting pairing. In ^{199}Hg , the most accurately measured isotope at present, we use $\bar{\beta}_3 = .09$, a phonon energy of 3 MeV (both taken from an E3 transition in ^{204}Hg , which may have a larger $\bar{\beta}_3$ than ^{199}Hg), and quadrupole and hexadecupole parameters from ref. [34] (for this simple estimate we ignore the fact that this nucleus is probably very soft). The resulting Schiff moment is $8 \times 10^{-9} \eta \text{ e fm}^3$, about half of the estimate from ref. [35] that includes no nuclear correlations of any kind. In a nucleus like this, moreover, with a relatively high-energy phonon, the nonaxial octupole vibrations will lie nearby in energy and can be expected to contribute comparable amounts. When all is said and done, vibrations may turn out to be the dominant contribution to the Schiff moment in ^{199}Hg , and they clearly should be included in any realistic calculation. Such a calculation has never been done, but is crucial if we want a reliable assessment of the advantages offered by nuclei with strong octupole correlations. Here we need a good microscopic treatment of all kinds of vibrations, including the very soft γ quadrupole mode, and must obviously go beyond mean-field theory. A shell-model calculation may be possible.

An example of a large vibrational Schiff moment is in the nucleus ^{239}Pu . This isotope has several features that make it attractive for experiment, in particular a spin-1/2 ground state (to eliminate quadrupole effects in a magnetic field) and a long half-life compared to the light actinides [The drawback is in its electronic structure, which is more complicated than that of Radium]. The collective E3 in ^{238}Pu gives $\beta_3 = .09$, and the nucleus has large quadrupole and hexadecupole deformations ($\beta_2 = .223$, $\beta_4 = .095$). Together with the high value of Z , this makes the intrinsic Schiff moment very large. The phonon lies at 470 keV, about 8 times higher than the lowest state in ^{225}Ra , but the large intrinsic Schiff moment compensates in part. Our calculations, with only the $\hat{\beta}$ -independent terms included in $\hat{\rho}$ (as in ref. [6]) give a laboratory Schiff moment of $7 \times 10^{-7} \eta \text{ e fm}^3$, a value a few times smaller than the results of ref. [6] for most of the light actinides. When we include the $\hat{\beta}$ -dependent terms, this number goes up to $4 \times 10^{-6} \eta \text{ e fm}^3$, which is 300 times the estimate for Hg in ref. [35] and comparable to the results of ref. [6] for ^{225}Ra . These calculations are far from perfect; we had to push the energy of the octupole phonon well above the value from ^{238}Pu to get the energy of the first excited state in ^{239}Pu right. The uncertainty in the results is therefore quite large and we need microscopic calculations here too. But the intrinsic Schiff moments will of nuclei with low-lying octupole vibrations will clearly

be collective, and some may of these nuclides may be easier to investigate experimentally than the short-lived Radium isotopes.

7 Conclusion

The size of Schiff moments in nuclei with octupole correlations is determined by three factors: intrinsic Schiff moments, energy denominators, and the matrix elements of \hat{V}_{PT} . In their discussion of the first two of these, refs. [5, 6] are on rather firm ground; it is hard to imagine, for example, that the matrix elements between parity doublets of the Schiff operator are radically different from those estimates, and as we have pointed out, even nuclei without asymmetrically deformed cores can benefit from the same mechanism. The third factor is far trickier, however.

The particle-core calculations reported both here and in earlier work can only supply a gross estimate of the matrix element of \hat{V}_{PT} . The mixing that that interaction induces depends sensitively on the valence single-particle wave function at the nuclear surface, where $\vec{\nabla}\rho$ is largest. Truly microscopic calculations will give better valence wave functions and, if they are self-consistent, will also better represent the correlation between density and mean field, and incorporate the effects of resonances caused by the residual interaction. In vibrational nuclei it will be necessary to go a little further, but even there mean-field calculations will shed light on the issues we've discussed.

Finally, for experimentalists to draw strong conclusions about enhancements over ^{199}Hg , better calculations in that nucleus must be done as well. It is conceivable that the atomic dipole moment of ^{225}Ra is 400 or more times larger than that of ^{199}Hg (this is the figure reported in ref. [6]), but we have pointed to physical effects that could make the Schiff moment in ^{199}Hg a few times larger than earlier calculations indicate and the Schiff moments in the light actinides somewhat smaller than suggested by the calculations of refs. [5, 6], even within the same model. The machinery of modern nuclear structure theory, which is powerful enough to provide reasonably accurate estimates of the moments in both kinds of nuclei, should be used as soon as possible to provide experimentalists firm predictions for the enhancement they can expect in difficult experiments with radioactive nuclei.

8 Acknowledgements

We thank J.L. Egido for useful calculations of Schiff moments in the even-even light actinides. We are grateful to W. Nazarewicz, I.B. Khriplovich, P. Herczeg, and S. Lamoreaux for helpful comments about the manuscript. The work of J.E. was supported by the U.S. Department of Energy under grant DE-FG02-97ER41019, and the work of J.L.F. and A.C.H. was performed under the auspices of the United States Department of Energy.

References

- [1] Robert G. Sachs, *The Physics of Time Reversal* (University of Chicago, 1987).

- [2] A. Angelopoulos et al., Phys. Lett. **B444**, 43 (1998).
- [3] I.B. Khriplovich and S.K. Lamoreaux, *CP Violation Without Strangeness: Electric Dipole Moments of Particles, Atoms, and Molecules* (Springer-Verlag, Berlin, Heidelberg, 1997).
- [4] W.C. Haxton and E.M. Henley, Phys. Rev. Lett. **51**, 1937 (1983).
- [5] N. Auerbach, V.V. Flambaum, and V. Spevak, Phys. Rev. Lett. **76**, 4316 (1996).
- [6] V. Spevak, N. Auerbach, and V. V. Flambaum, Phys. Rev. C **56**, 1357 (1997).
- [7] I.B. Khriplovich, *Parity Nonconservation in Atomic Phenomena* (Gordon and Breach, New York, 1991).
- [8] O.P. Sushkov, V.V. Flambaum, and I.B. Khriplovich, Zh. Exp. Teor. Fiz. **87**, 1521, 1984 [Sov. Phys. JETP **60**, 873 (1984)].
- [9] R.P. Feynman, Phys. Rev. **56**, 340 (1939); H. Hellmann, *Einführung in die Quantumchemie* (Franz Deuticke, Leipzig, 1937), p. 285. The usual statement of the theorem is that if a Hamiltonian $H(\lambda)$ depends on a parameter λ , the energy shift $E(\lambda)$ for that Hamiltonian satisfies $\frac{\partial E(\lambda)}{\partial \lambda} = \langle \Psi(\lambda) | \frac{\partial H(\lambda)}{\partial \lambda} | \Psi(\lambda) \rangle$. If one performs a unitary transformation so that $H(\lambda) = \exp(i\lambda U) H(0) \exp(-i\lambda U)$, uses the theorem and then sets λ to zero, one finds $\frac{\partial E(0)}{\partial \lambda} \equiv 0 = i\langle [U, H(0)] \rangle$, since there can be no energy shift from a unitary transformation. Our quantity Δ in eqs. (6) and (21) is given by this relationship.
- [10] V. Fock, Z. Phys. **63**, 855 (1930).
- [11] E. M. Purcell and N. F. Ramsey, Phys. Rev. **78**, 807 (1950).
- [12] L.I. Schiff, Phys. Rev. **132**, 2194 (1963).
- [13] J.L. Friar, Few-Body Systems **22**, 161 (1997).
- [14] S.T. Epstein and J.O. Hirschfelder, Phys. Rev. **123**, 1495 (1961).
- [15] J.L. Friar and S. Fallieros, Phys. Lett. **114B**, 403 (1982). Although no consensus notation for retarded electric multipoles exists, we adopt the nomenclature of this reference, which has seen considerable use.
- [16] J. Goldemberg, Y. Torizuka, W.C. Barber, and J.D. Walecka, Nucl. Phys. **43**, 242 (1963).
- [17] R.M. Wilcox, J. Math. Phys. **8**, 962 (1967) derives and discusses various forms of the Baker-Campbell-Hausdorff (BCH) formula (including eq. (4.15) that we require). Fourier transforming eq. (28) leads to $\hat{F}_{\text{GT}}(\vec{k}) = F_0(k^2) \exp(i\vec{k} \cdot \vec{q} N/A) = F_0(k^2) \exp(i\xi^\dagger + i\xi)$, where $\xi = (N\vec{k} \cdot \vec{a}/A)(\hbar/2\mu\omega)^{1/2}$ and F_0 is the Fourier transform of ρ_0 . Because $[\xi, \xi^\dagger] = N^2 \hbar k^2 / 2\mu\omega A^2$ is a c-number, one obtains the exact BCH

result, $\hat{F}_{\text{GT}}(\vec{k}) = F_{\text{ch}}(k^2) \exp(i\xi^\dagger) \exp(i\xi)$, where the exact ground-state charge form factor for the GT model is given by $F_{\text{ch}}(k^2) = F_0(k^2) \exp(-N^2 \hbar k^2 / 2\mu\omega A^2)$, since $\langle \hat{F}_{\text{GT}} \rangle = F_{\text{ch}}$ follows from $\xi|0\rangle = 0$. It also follows that all excitations are determined by ρ_{ch} (the inverse transform of F_{ch}) instead of ρ_0 . This simple modification accounts for all vacuum fluctuations in the GT model.

- [18] D.M. Brink, Nucl. Phys. **4**, 215 (1957).
- [19] A. Arima, P. Manakos, and D. Strottman, Phys. Lett. **B60**, 1 (1975).
- [20] D. Agassi, V. Gillet, and A. Lumbroso, Nucl. Phys. **A144**, 161 (1970).
- [21] D.J. Millener, A.C. Hayes, and D. Strottman, Phys. Rev. C **45**, 473 (1992).
- [22] Malcolm Harvey, Advances in Nucl. Phys. Vol **1** 67, (1968).
- [23] P.A. Butler and W. Nazarewicz, Rev. Mod. Phys. **68**, 349 (1996).
- [24] I.S. Towner and A.C. Hayes, Phys. Rev. C **49**, 2391 (1994).
- [25] A. Griffiths and P. Vogel, Phys. Rev. C **43**, 2844 (1991).
- [26] P. Herczeg, Hyperfine Interactions **43**, 77 (1988).
- [27] A. Bohr and B. Mottelson, *Nuclear Structure* (Benjamin, New York, 1975), Vol. 2.
- [28] G.A. Leander, W. Nazarewicz, G.F. Bertsch, and J. Dudek, Nucl. Phys. **A453**, 58 (1986)
- [29] J.L. Egido and L.M. Robledo, Nucl. Phys. **A545**, 589 (1992), and references therein.
- [30] V. Martín and L.M. Robledo, Phys. Rev. C **49**, 188 (1994); Phys. Rev. C **50**, 520 (1994).
- [31] J.L. Egido, private communication.
- [32] R.H. Spear, At. Dat. Nucl. Dat. Tables **42**, 55 (1989).
- [33] G.A. Leander and R.K. Sheline, Nucl. Phys. **A413**, 375 (1991).
- [34] P. Moller, R. Nix, W.D. Myers, et al., At. Data Nucl. Data Tables **59**, 185 (1995).
- [35] V.V. Flambaum, I.B. Khriplovich, and O.P. Sushkov, Nucl. Phys. **A449**, 750 (1986)